On the Matrix Representation of Quantum Operations

Yoshihiro Nambu and Kazuo Nakamura Fundamental and Environmental Research Laboratories, NEC, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, Japan (Dated: February 1, 2008)

This paper considers two frequently used matrix representations — what we call the χ - and \mathcal{S} -matrices — of a quantum operation and their applications. The matrices defined with respect to an arbitrary operator basis, that is, the orthonormal basis for the space of linear operators on the state space are considered for a general operation acting on a single or two d-level quantum system (qudit). We show that the two matrices are given by the expansion coefficients of the Liouville superoperator as well as the associated bijective, positive operator on the doubled-space defined with respect to two types of induced operator basis having different tensor product structures, i.e., Kronecker products of the relevant operator basis and dyadic products of the associated bipartite state basis. The explicit conversion formulas between the two matrices are established as a computable matrix multiplication. Extention to more qudits case is trivial. Several applications of these matrices and the conversion formulas in quantum information science and technology are presented.

PACS numbers: 03.67.-a, 03.65.Wj

I. INTRODUCTION

The formalism of quantum operations offers us a powerful tool for describing the dynamics of quantum systems occurring in quantum computation, including unitary evolution as well as non-unitary evolution [1, 2]. It can deal with several central issues: measurements in the middle of the computation, decoherence and noise, using probabilistic subroutines, etc. [3]. It describes the most general transformation allowed by quantum mechanics for an initially isolated quantum system [4, 5]. Experimental characterization and analysis of quantum operations is an essential component of on-going efforts to develop devices capable of reliable quantum computing and quantum communications, and is a research subject of considerable recent interest. There have been extensive efforts on the statistical estimation of quantum operations occurring in natural or engineered quantum processes from experimental data known as "quantum channel identification" or "quantum process tomography" [6, 7, 8, 9, 10, 11, 12].

There are several ways of introducing the notion of a quantum operation, one of which is to consider it as superoperators acting on the space of linear operators [3, 13, 14]. Any physical quantum operation has to be described by a superoperator that is completely positive (CP); i.e., it should map the set of density operators acting on the trivially extended Hilbert space to itself [1, 2]. It is known that any CP map can be decomposed into the so-called Kraus form by a set of Kraus operators [1]. However, this description is unique only up to unitary equivalence [2], just like the decomposition of a given density operator into convex sum of distinct, but not necessarily orthogonal, projectors is unique only up to unitary equivalence [2, 15]. Alternatively, the superoperators can be represented in matrix form by providing an operator basis [16], i.e., the orthonormal basis for the space of linear operators on the state space, just as the operators on the Hilbert space can be represented in matrix form by providing a state basis for the Hilbert space. For example, the density operator can be represented by a density matrix defined with respect to the chosen state basis. The density matrix provides a unique description of the quantum state once the state basis is fixed, although we still have a freedom in choosing the state basis. Similarly, a quantum operation can also be uniquely described using the matrix once the operator basis has been fixed.

One can construct many different types of matrix representation. This paper considers two different matrix representations for superoperators frequently found in the literature. The first one is what we call the χ -matrix, which is also called the process or dynamical matrix by several authors [2, 7, 10, 12, 17, 19, 20]. Let us consider a d-dimensional Hilbert space (H-space) \mathcal{H}_d , and the space of linear operators acting on \mathcal{H}_d with a scalar product $\langle \hat{A}, \hat{B} \rangle \equiv \text{Tr} \hat{A}^{\dagger} \hat{B}$, that is, the Hilbert-Schmidt space (HS-space) \mathcal{HS}_d . If we choose the fixed basis set $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ in \mathcal{HS}_d , the linear operation \mathfrak{S} can be represented by the binary form of the superoperator

$$\hat{\hat{\mathcal{S}}}(\odot) = \sum_{\alpha,\beta=0}^{d^2-1} \chi_{\alpha\beta} \hat{E}_{\alpha} \odot \hat{E}_{\beta}^{\dagger}$$
 (1)

acting on \mathcal{HS}_d , which maps a linear operator in \mathcal{HS}_d into another one. In Eq. (1), the substitution symbol \odot should be replaced by a transformed operator, and double-hat $\hat{}$ is used to distinguish the superoperator from an ordinary operator acting on \mathcal{H}_d . The coefficients $\chi_{\alpha\beta}$ form a $d^2 \times d^2$ positive matrix $\chi \equiv [\chi_{\alpha\beta}]_{\alpha,\beta=0}^{d^2-1}$, if \mathfrak{S} is a physical quantum operation [21].

Alternatively, another matrix representation of a quantum operation is given in terms of the Liouville formalism [13, 22, 23]. In this formalism, the linear operators in \mathcal{HS}_d are identified with the supervectors in a Liouville space (*L*-space) \mathcal{L}_{d^2} . Introducing a double bra-ket

notation for the elements of \mathcal{L}_{d^2} [23], we associate every operator \hat{A} with an L-ket $|\hat{A}\rangle\rangle$ and its Hermitian conjugate operator \hat{A}^{\dagger} with an L-bra $\langle\langle\hat{A}|$. The space \mathcal{L}_{d^2} is furnished with an inner product $\langle\langle\hat{A}|\hat{B}\rangle\rangle=\mathrm{Tr}\hat{A}^{\dagger}\hat{B}$, and constitutes a d^2 -dimensional Hilbert space. Then by chosing an arbitrary fixed set of operator basis $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ in \mathcal{HS}_d , any linear operation \mathfrak{S} can be written as the superoperator

$$\hat{\hat{\mathcal{S}}} = \sum_{\alpha,\beta=0}^{d^2-1} \mathcal{S}_{\alpha\beta} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|$$
 (2)

acting on \mathcal{L}_{d^2} , which maps a L-space supervector into another one. The coefficients $\mathcal{S}_{\alpha\beta}$ form a $d^2 \times d^2$ complex matrix $\mathcal{S} \equiv [\mathcal{S}_{\alpha\beta}]_{\alpha,\beta=0}^{d^2-1}$. They represent the amplitudes of the operator components \hat{E}_{α} contained in the state after applying the quantum operation on the operator component \hat{E}_{β} . We call it the \mathcal{S} -matrix by analogy with the S-matrix appearing in time-independent scattering theory [24, 25]. The \mathcal{S} -matrix has been actually used to describe quantum operations by several researchers on quantum information science [8, 9, 26]. The χ - and \mathcal{S} -matrices offer us the most general description of the dynamics of initially isolated quantum systems allowed in quantum mechanics, just as the density matrix offers us the most general description of the quantum mechanical state.

The choice of matrix representation type is a matter of convenience, depending on the application. We will discuss later how the χ - and S-matrices are useful for the analysis and design of quantum operations. Although these matrices indeed have their own useful applications. their mutual relation is non-trivial and has not been clarified. The main purpose of this paper is to clarify the underlying relation between two different matrix representations of quantum operations, and to provide the way for building bridges across the different classes of applications. We here consider a quantum operation acting on the state of a single d-level quantum system (abbreviated as single-qudit operation) or a two d-level quantum systems (two-qudit operation). We start in Sec. II by recalling the notion of operator basis and its properties, which is helpful for the subsequent discussions. We note the equivalence between the supervectors in the Lspace \mathcal{L}_{d^2} and the vectors in the doubled Hilbert space $\mathcal{H}_d^{\otimes 2} = \mathcal{H}_d \otimes \mathcal{H}_d$. This equivalence implies that for any operator-basis set $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ for \mathcal{HS}_d , there is an isomorphic state-basis set $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ for $\mathcal{H}_d^{\otimes 2}$. We review several properties of the operator basis for later discussion. In Sec. III, we first consider the single-qudit operations. We show that χ - and S-matrices are given by the expansion coefficients of the L-space superoperator \hat{S} and the associated operator $\hat{\chi} \equiv \hat{\mathcal{S}} \otimes \hat{\mathcal{I}}(d\hat{\rho}_I)$ acting on $\mathcal{H}_d^{\otimes 2}$ defined with respect to two types of induced operator basis on $\mathcal{H}_d^{\otimes 2}$ having different tensor product structures. Here, $\hat{\rho}_I$ is the density operator of the isotropic state

on $\mathcal{H}_{d}^{\otimes 2}$, and $\hat{\mathcal{I}}(\odot) = \odot$ is the identity superoperator acting on the HS-space of the second system. This result implies that there is a bijection between \hat{S} and $\hat{\chi}$, from which we can deduce the conversion formula between χ - and S-matrices as a computable matrix algebra. Although Nielsen and Chuang have considered such a formula [2, 17], their method requires finding matrix inverses to convert from the S-matrix to the χ -matrix. Here, we show a conversion formula without matrix inversion. We then extend the formula to two-qudit operations. We also briefly review the requirement for the χ -matrix to represent physical operations. In Sec. IV, we illustrate the applications of the present formulation. First, we discuss how χ - and S-matrices can be obtained experimentally. We describe a typical procedure to obtain the χ - and S-matrices defined with respect to an arbitrary operator basis set. Next, we discuss how these matrices and the present conversion formulas are useful for the analysis and design of the quantum operations, quantum circuits, as well as quantum algorithms. In Sec. V, we summarize the results.

II. OPERATOR BASIS

It has been noted by many researchers that the supervectors defined in the L-space \mathcal{L}_{d^2} can be identified with the vectors in the doubled Hilbert space $\mathcal{H}_d^{\otimes 2}$ [27, 28, 29, 30]. Let us start by reviewing this fact, briefly. Consider an arbitrary chosen set of an orthonormal basis $\{|i\rangle\}_{i=1}^{d-1}$ for \mathcal{H}_d (denoted as standard state basis). Any linear operator \hat{A} in \mathcal{HS}_d can be expanded as $\hat{A} = \sum_{i,j=0}^{d-1} A_{ij} |i\rangle\langle j|$ where the dyadic products $|i\rangle\langle j|$ form a basis for \mathcal{HS}_d . The L-space supervectors corresponding to the dyadic operator $|i\rangle\langle j|$ is denoted by the double ket $|ij\rangle\rangle$, with which the L-space supervector associated with \hat{A} is written as $|\hat{A}\rangle\rangle = \sum_{i,j=0}^{d-1} A_{ij} |ij\rangle\rangle$. The scalar product of two L-space supervectors $|\hat{A}\rangle\rangle$ and $|\hat{B}\rangle\rangle$ is defined as

$$\langle \langle \hat{A} | \hat{B} \rangle \rangle = \text{Tr} \hat{A}^{\dagger} \hat{B},$$
 (3)

which introduces a metric of an L-space. The vectors $|ij\rangle\rangle$ form a basis for a d^2 -dimensional Hilbert space. Thus, we can safely identify $|ij\rangle\rangle$ with the product state $|i\rangle\otimes|j\rangle$. Then, the L-space vector associated with \hat{A} can be identified with vector $|\hat{A}\rangle\rangle\equiv(\hat{A}\otimes\hat{I})|\hat{I}\rangle\rangle$ in the doubled space $\mathcal{H}_d^{\otimes 2}[21,\ 31]$, where $d^{-1/2}|\hat{I}\rangle\rangle\equiv d^{-1/2}\sum_{i=0}^{d-1}|i\rangle\otimes|i\rangle$ is the isotropic state in $\mathcal{H}_d^{\otimes 2}$ [32, 33], and \hat{I} is the identity operator in \mathcal{HS}_d . It may be helpful to recall the mathematical representations of \hat{A} in the space $\mathbb{C}^{d\times d}$ of $d\times d$ complex matrices and the vector $|\hat{A}\rangle\rangle$ in \mathbb{C}^{d^2} . Consider a representation where $|i\rangle$ is a column vector in \mathbb{C}^d with a unit element in the jth row and zeros elsewhere. Then, \hat{A} is identified with the $d\times d$ complex matrix $A\equiv [A_{ij}]_{i,j=0}^{d-1}$ in $\mathbb{C}^{d\times d}$, and $|\hat{A}\rangle\rangle$ is obtained by placing the entries of a

 $d \times d$ matrix into a column vector of size d^2 row-by-row, i.e.,

$$|\hat{A}\rangle\rangle \equiv [A_{11}, \cdots, A_{1d}, A_{21}, \cdots, A_{2d}, \cdots, A_{d1}, \cdots, A_{dd}]^T.$$
(4)

Therefore, $|\hat{A}\rangle\rangle$ contains the same elements as \hat{A} but in different positions. This and Eq. (3) indicate that \hat{A} and $|\hat{A}\rangle\rangle$ are isometrically isomorphic. Accordingly, we may identify the L-space with the doubled Hilbert space, i.e., $\mathcal{L}_{d^2} = H_d^{\otimes 2}$. Hereafter, we use a common symbol $\mathcal{H}_d^{\otimes 2}$ to denote both these spaces without loss of clarity.

It will be useful for the later discussion to note the following relations hold:

$$\hat{A} \otimes \hat{B} |\hat{C}\rangle\rangle = |\hat{A}\hat{C}\hat{B}^T\rangle\rangle,$$
 (5)

$$Tr_2[|\hat{A}\rangle\rangle_{12} \langle\langle \hat{B}|] = (\hat{A}\hat{B}^{\dagger})^{(1)}, \tag{6}$$

$$Tr_1[|\hat{A}\rangle\rangle_{12^{12}}\langle\langle\hat{B}|] = (\hat{A}^T\hat{B}^*)^{(2)},$$
 (7)

where the indices refer to the factors in $\mathcal{H}_d^{\otimes 2}$ in which the corresponding operators have a nontrivial action, and the transposition and conjugation are referred to the chosen standard state basis [16].

Now, let us consider the operator basis, that is, the complete basis for \mathcal{HS}_d . Consider an arbitrary set of d^2 -vectors in $\mathcal{H}_d^{\otimes 2}$. From the above isomorphism, this set can be written as $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$, where $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ is the associated set in \mathcal{HS}_d . The set $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ is the state basis for $\mathcal{H}_d^{\otimes 2}$ iff it is orthonormal, i.e.,

$$\langle\langle \hat{E}_{\alpha}|\hat{E}_{\beta}\rangle\rangle = \delta_{\alpha\beta},$$
 (8)

and it is complete, i.e.,

$$\sum_{\alpha=0}^{d^2-1} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\alpha}| = \hat{I} \otimes \hat{I}. \tag{9}$$

The previous discussion shows that the vector $|\hat{A}\rangle\rangle$ in $\mathcal{H}_d^{\otimes 2}$ is identified with *L*-space supervectors associated with the operator \hat{A} in \mathcal{HS}_d . This implies the following proposition.

Proposition 1 A set of the operators $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ is a basis set for \mathcal{HS}_d iff a set of states $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ is the basis set for $\mathcal{H}_d^{\otimes 2}$.

We argue below that this is true. First, we note the following lemmmas.

Lemma 1 A set of the operators $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ in \mathcal{HS}_d is orthonormal iff a set of states $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ in $\mathcal{H}_d^{\otimes 2}$ is orthonormal.

This is a trivial consequence of Eq. (3).

Lemma 2 A set of the operators $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ in \mathcal{HS}_d is complete iff a set of states $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ in $\mathcal{H}_d^{\otimes 2}$ is complete.

To prove this, the following Theorem is helpful [16]:

Theorem 1 (D'Ariano, Presti, and Sacchi (2000)) A set of the operators $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ in \mathcal{HS}_d is complete iff it satisfies one of the following equivalent statements:

1. For any linear operator \tilde{A} on \mathcal{H}_d , we have

$$\hat{A} = \sum_{\alpha=0}^{d^2 - 1} (\operatorname{Tr} \hat{E}_{\alpha}^{\dagger} \hat{A}) \hat{E}_{\alpha}. \tag{10}$$

2. Let $\hat{\mathcal{E}}_{depol}(\cdots)$ be the superoperator on the space of linear operators in \mathcal{HS}_d describing completely depolarizing operation. For any linear operator \hat{A} on \mathcal{H}_d , we have

$$\hat{\mathcal{E}}_{depol}(\hat{A}) = \frac{1}{d} (\operatorname{Tr} \hat{A}) \hat{I} = \frac{1}{d} \sum_{\alpha=0}^{d^2 - 1} \hat{E}_{\alpha} \hat{A} \hat{E}_{\alpha}^{\dagger}. \tag{11}$$

3. For chosen any state basis $\{|i\rangle\}_{i=1}^{d-1}$ for \mathcal{H}_d , we have

$$\sum_{\alpha=0}^{d^2-1} \langle n|\hat{E}_{\alpha}^{\dagger}|m\rangle\langle l|\hat{E}_{\alpha}|k\rangle = \delta_{nk}\delta_{ml}.$$
 (12)

Now, let us prove Lemma 2. If $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ is complete, Eq. (9) must be satisfied. Then, for any \hat{A} in \mathcal{HS}_d , we have

$$\begin{split} (\hat{A} \otimes \hat{I})|\hat{I}\rangle\rangle &= |\hat{A}\rangle\rangle \ = \ \sum_{\alpha=0}^{d^2-1} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\alpha}|\hat{A}\rangle\rangle \\ &= \ \sum_{\alpha=0}^{d^2-1} (\mathrm{Tr}\hat{E}_{\alpha}^{\dagger}\hat{A})\hat{E}_{\alpha} \otimes \hat{I}|\hat{I}\rangle\rangle. \end{split}$$

Since this holds for any \hat{A} , Eq. (10) must be satisfied. Hence, $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ is complete. Conversely, if $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ is complete, then for any $|\hat{A}\rangle$ in $\mathcal{H}_d^{\otimes 2}$, we have

$$|\hat{A}\rangle\rangle = (\hat{A} \otimes \hat{I})|\hat{I}\rangle\rangle = \sum_{\alpha=0}^{d^2-1} (\operatorname{Tr}\hat{E}_{\alpha}^{\dagger}\hat{A})\hat{E}_{\alpha} \otimes \hat{I}|\hat{I}\rangle\rangle$$
$$= \sum_{\alpha=0}^{d^2-1} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\alpha}|\hat{A}\rangle\rangle.$$

Since this holds for any $|\hat{A}\rangle\rangle$, Eq. (9) must be satisfied. Hence, $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ is complete. From these two lemmas, we obtain Proposition 1. This indicates that the state basis $|\hat{E}_{\alpha}\rangle\rangle$ for $\mathcal{H}_{d}^{\otimes 2}$ has bijective correspondence to the operator basis \hat{E}_{α} for \mathcal{HS}_{d} . The following corollary is a consequence of Theorem 1, which will be useful for the later discussions.

Corollary 1 Let $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ be an arbitrary chosen set of an operator basis for \mathcal{HS}_d . The isotropic state in $\mathcal{H}_d^{\otimes 2}$ is written as

$$\hat{\rho}_I = \frac{1}{d} |\hat{I}\rangle\rangle\langle\langle\hat{I}| = \frac{1}{d} \sum_{\alpha=0}^{d^2 - 1} \hat{E}_\alpha \otimes \hat{E}_\alpha^*, \tag{13}$$

and the swap operator \hat{V} on $\mathcal{H}_d^{\otimes 2}$ is written as

$$\hat{V} = \sum_{\alpha=0}^{d^2 - 1} \hat{E}_{\alpha} \otimes \hat{E}_{\alpha}^{\dagger}. \tag{14}$$

Equation (13) can be proven by explicit evaluation of the matrix elements and using Eq. (12). Equation (14) is obtained by performing the partial transpose on both sides of Eq. (13) with respect to the second system.

Examples of the operator basis

We show three illustrative examples of the operator basis for \mathcal{H}_d frequently found in the literature. The first example is a set of transition operators $\hat{\pi}_{(i,j)} :=$ $|i\rangle\langle j|$ with $i,j=0,\cdots,d-1$, and (i,j):=di+j[34]. The associated states form a basis set $\{|\hat{\pi}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ whose elements are the tensor product of the standard state basis, i.e., $|\hat{\pi}_{(i,j)}\rangle\rangle = |i\rangle\otimes|j\rangle$. The next example is a set of unitary irreducible representations of the group SU(d) or the discrete displacement operators on the phase-space torus, whose elements are $\hat{U}_{(m,n)} =$ $\omega^{mn/2} \sum_{k=0}^{d-1} \omega^{mk} \hat{\pi}_{(k \oplus n,k)} / \sqrt{d}$ with $m, n = 0, \dots, d-1$, where $\omega = 1^{1/d} = e^{i2\pi/d}$ and \oplus denotes addition modulo d [34, 35, 36]. The associated states form a basis set $\{|\hat{U}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ of d^2 -orthogonal maximally entangled states in $\mathcal{H}_d^{\otimes 2}$. The last example is a set of d^2-1 traceless Herical mitian generators of the group SU(d) supplemented with the normalized identity operator given by $\{\hat{\lambda}_{\alpha}\}_{\alpha=0}^{d^2-1} =$ $\{\hat{I}/\sqrt{d}, \hat{u}_{0,1}, \hat{u}_{0,2}, \cdots, \hat{u}_{d-2,d-1}, \hat{v}_{0,1}, \hat{v}_{0,2}, \cdots, \hat{v}_{d-2,d-1},$ $\hat{w}_1, \hat{w}_2, \cdots, \hat{w}_{d-1}$ } where d(d-1) off-diagonal generators are given by $\hat{u}_{i,j} = (\hat{\pi}_{(i,j)} + \hat{\pi}_{(j,i)})/\sqrt{2}, \ \hat{v}_{i,j} =$ $i(\hat{\pi}_{(i,j)} - \hat{\pi}_{(j,i)})/\sqrt{2}$ with $0 \le i < j \le d-1$, and d-1 diagonal generators are given by $\hat{w}_k =$ $(-\sum_{i=0}^{k-1} \hat{\pi}_{(i,i)} + k\hat{\pi}_{(k,k)})/\sqrt{k(k+1)}$ with $1 \leq k \leq d-1$ [34]. The choice of basis is of course a matter of convenience, depending on the application.

Since the associated sets $\{|\hat{\pi}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$, $\{|\hat{U}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$, and $\{|\hat{\lambda}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ are state bases for $\mathcal{H}_d^{\otimes 2}$, they should be unitarily related. This implies that the operator bases $\hat{\pi}_{\alpha}$, \hat{U}_{α} , and $\hat{\lambda}_{\alpha}$ should also be unitarily related. In general, two sets of state basis $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ and $\{|\hat{F}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ in

 $\mathcal{H}_d^{\otimes 2}$ are unitarily related, i.e.,

$$|\hat{F}_{\beta}\rangle\rangle = \sum_{\alpha=0}^{d^2-1} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\alpha}|\hat{F}_{\beta}\rangle\rangle = \sum_{\alpha=0}^{d^2-1} |\hat{E}_{\alpha}\rangle\rangle\mathcal{U}_{\alpha\beta} \qquad (15)$$

iff the operator bases \hat{E}_{α} and \hat{F}_{α} in \mathcal{HS}_d are unitarily related, i.e.,

$$\hat{F}_{\beta} = \sum_{\alpha=0}^{d^2 - 1} \hat{E}_{\alpha} \mathcal{U}_{\alpha\beta}.$$
 (16)

In Eqs. (15) and (16), $\mathcal{U}_{\alpha\beta} = \langle \langle \hat{E}_{\alpha} | \hat{F}_{\beta} \rangle \rangle = \text{Tr} \hat{E}_{\alpha}^{\dagger} \hat{F}_{\beta}$ is a $\alpha\beta$ -entry of the $d^2 \times d^2$ unitary matrix \mathcal{U} . If we consider a unitary superoperator acting on the vectors in $\mathcal{H}_d^{\otimes 2}$,

$$\hat{\hat{\mathcal{U}}} = \sum_{\alpha,\beta=0}^{d^2-1} \mathcal{U}_{\alpha\beta} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|, \tag{17}$$

Equations. (15) and (16) are the unitary transformation of the operators. Note that Eq. (16) does not imply unitary equivalence of \hat{E}_{α} and \hat{F}_{α} , i.e., $\hat{F}_{\beta} = \hat{W} \hat{E}_{\alpha} \hat{W}^{\dagger}$ for some unitary operator \hat{W} in \mathcal{HS}_d , although the unitary equivalence of \hat{E}_{α} and \hat{F}_{α} implies Eq. (16). In general, $\hat{F}_{\beta} \neq \hat{W} \hat{E}_{\alpha} \hat{W}^{\dagger}$ for any unitary operator \hat{W} in \mathcal{HS}_d , even if Eq. (16) holds. For example, $\hat{\pi}_{(i,j)}$ is the operator basis of all the elements of which have rank one, whereas \hat{U}_{α} and $\hat{\lambda}_{\alpha}$ are those operator bases of all the elements of which have rank exceeding one. Therefore, $\hat{\pi}_{(i,j)}$ is induced by a standard state basis $\{|i\rangle\}_{i=0}^{d-1}$ for \mathcal{H}_d , whereas \hat{U}_{α} and $\hat{\lambda}_{\alpha}$ are not. This clearly indicates that either the set $\{\hat{U}_{\alpha}\}_{\alpha=0}^{d^2-1}$ or $\{\hat{\lambda}_{\alpha}\}_{\alpha=0}^{d^2-1}$ is unitarily related to the set $\{\hat{\pi}_{\alpha}\}_{\alpha=0}^{d^2-1}$, but is not unitarily equivalent to this set.

III. MATRIX REPRESENTATION OF QUANTUM OPERATIONS

Let us turn our attention to a single-qudit operation. As shown in Sec. I, this quantum operation can be represented by either an HS-space superoperator or an L-space superoperator, in which the χ - and S-matrices are introduced with respect to the arbitrary, but associated sets of basis $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ for \mathcal{HS}_d and $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$ for $\mathcal{H}_d^{\otimes 2}$, respectively. In this section, the underlying relationship between these two matrix representations is discussed.

Let us first consider the L-space superoperator. In the Liouville formalism, the operators in \mathcal{HS}_d are identified with the vectors in $\mathcal{H}_d^{\otimes 2}$. Any operation \mathfrak{S} is identified with the one-sided operator $\hat{\mathcal{S}}$ acting on $\mathcal{H}_d^{\otimes 2}$, which can be expanded using the state basis $|\hat{E}_{\alpha}\rangle$ for $\mathcal{H}_d^{\otimes 2}$ as shown in Eq. (2). The elements of a $d^2 \times d^2$ matrix \mathcal{S} are formally written as $\mathcal{S}_{\alpha\beta} = \langle \langle \hat{E}_{\alpha} | \hat{\mathcal{S}} | \hat{E}_{\beta} \rangle \rangle$. Alternatively, the same operation \mathfrak{S} is written as a two-sided superoperator acting on the operator in \mathcal{HS}_d , which can be expanded

using the operator basis \hat{E}_{α} for \mathcal{HS}_d as shown in Eq. (1). Since $\hat{S}|\hat{E}_{\beta}\rangle\rangle = |\hat{S}(\hat{E}_{\beta})\rangle\rangle$, we find the matrix element $S_{\alpha\beta}$ can also be written as

$$S_{\alpha\beta} = \langle \langle \hat{E}_{\alpha} | \hat{\hat{S}}(\hat{E}_{\beta}) \rangle \rangle = \sum_{\gamma, \delta = 0}^{d^2 - 1} \chi_{\gamma\delta} \langle \langle \hat{E}_{\alpha} | \hat{E}_{\gamma} \otimes \hat{E}_{\delta}^* | \hat{E}_{\beta} \rangle \rangle,$$
(18)

where we used Eq. (5). Substituting the right-hand side of Eq. (18) for $S_{\alpha\beta}$ in Eq. (2), we find that \hat{S} can be written in terms of either the matrix S or χ as

$$\hat{\hat{\mathcal{S}}} = \sum_{\alpha,\beta=0}^{d^2-1} \mathcal{S}_{\alpha\beta} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}| = \sum_{\alpha,\beta=0}^{d^2-1} \chi_{\alpha\beta} \hat{E}_{\alpha} \otimes \hat{E}_{\beta}^*. \quad (19)$$

In Eq. (19), we find two types of induced operator basis on $\mathcal{H}_d^{\otimes 2}$ having different tensor product structures, that is, Kronecker products $\hat{E}_{\alpha} \otimes \hat{E}_{\beta}^*$ and dyadic products $|\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|$ of the state basis associated with the operator basis set $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$. Note that both types of basis set do not cover all the possible basis sets on $\mathcal{H}_d^{\otimes 2}$. Obviously, the former type of basis set covers only those sets that are factorable with respect to the original and extended system spaces. For example, the set of d^4 -dyadic products of the d^2 -maximally-entangled states in $\mathcal{H}_d^{\otimes 2}$ is not a factorable basis set, and can not be covered by the former type. Similarly, only an operator basis on $\mathcal{H}_d^{\otimes 2}$ with all elements of which have rank one can be reduced to the latter type of the basis set. Therefore, each type of basis set can describe its own particular subset of all the possible basis sets on $\mathcal{H}_d^{\otimes 2}$.

Let us next consider another operator $\hat{\chi}$ on $\mathcal{H}_d^{\otimes 2}$, which we call the Choi operator [37]. We will show that this operator has bijective correspondence to the L-space superoperator $\hat{\mathcal{S}}$. It is known that the isomorphism between the operator in \mathcal{HS}_d and the bipartite vector in $\mathcal{H}_d^{\otimes 2}$ can be straightforwardly extended to the isomorphism between the superoperator acting on \mathcal{HS}_d and the operator acting on $\mathcal{H}_d^{\otimes 2}$. Jamiołkowski first showed that the map between the HS-space superoperator $\hat{\mathcal{S}}(\odot)$ and the operator $\hat{\mathcal{S}}(\odot)$ and $\hat{\mathcal{T}}(d\hat{\rho}_I)$ acting on $\mathcal{H}_d^{\otimes 2}$ is an isomorphism, where $\hat{\mathcal{S}}(\odot)$ and $\hat{\mathcal{T}}(\odot)$ act on the HS-space of the first and second systems, respectively [38]. If we note Eq. (13) and the following equivalent relation that follows from Eq. (19)

$$|\hat{\hat{\mathcal{S}}}|\hat{E}_{\beta}\rangle\rangle = \sum_{\alpha=0}^{d^2-1} \mathcal{S}_{\alpha\beta}|\hat{E}_{\alpha}\rangle\rangle \leftrightarrow \hat{\hat{\mathcal{S}}}(\hat{E}_{\beta}) = \sum_{\alpha=0}^{d^2-1} \mathcal{S}_{\alpha\beta}\hat{E}_{\alpha},$$

it is easy to confirm that $\hat{\chi}$ can be written as

$$\hat{\chi} = \sum_{\alpha,\beta=0}^{d^2-1} \chi_{\alpha\beta} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}| = \sum_{\alpha,\beta=0}^{d^2-1} \mathcal{S}_{\alpha\beta} \hat{E}_{\alpha} \otimes \hat{E}_{\beta}^*. \quad (20)$$

Equations (19) and (20) are one of the main results of this paper. From these equations, we find that $\hat{\mathcal{S}}$ and $\hat{\chi}$ are complementary to each other in the sense that they can be interchanged if we exchange the two operator bases $|\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|$ and $\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*}$ on $\mathcal{H}_{d}^{\otimes 2}$ in their expressions. These equations show that the \mathcal{S} -matrix (χ -matrix) is given by the expansion coefficients of $\hat{\mathcal{S}}$ ($\hat{\hat{\chi}}$) with respect to $|\hat{E}_{\alpha}\rangle\rangle\langle\langle\langle\hat{E}_{\beta}|$ as well as those of $\hat{\chi}$ ($\hat{\mathcal{S}}$) with respect to $\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*}$, which is explicitly written as

$$\chi_{\alpha\beta} = \text{Tr}(|\hat{E}_{\alpha}\rangle)\langle\langle\hat{E}_{\beta}|)^{\dagger}\hat{\hat{\chi}} = \text{Tr}(\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*})^{\dagger}\hat{\hat{S}}, \qquad (21)$$

$$S_{\alpha\beta} = \text{Tr}(|\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|)^{\dagger}\hat{S} = \text{Tr}(\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*})^{\dagger}\hat{\chi}.$$
 (22)

From Eqs. (19) and (20), we can explore the mutual conversion formulas between χ - and \mathcal{S} -matrices. To this end, let us define a bijection between the two operators on $\mathcal{H}_d^{\otimes 2}$ originally found by Havel [40].

$$\Lambda(\odot) = \sum_{\gamma=0}^{d^2-1} (\hat{I} \otimes \hat{\pi}_{\gamma}) \odot (\hat{\pi}_{\gamma} \otimes \hat{I}), \tag{23}$$

which is also considered to be the super-superoperator acting on \mathcal{H}_d . Then, we have the following Theorem [40].

Theorem 2 (Havel (2003)) For arbitrary operators \hat{X} and \hat{Y} in \mathcal{HS}_d , we have

$$|\hat{X}\rangle\rangle\langle\langle\hat{Y}| = \Lambda(\hat{X}\otimes\hat{Y}^*),$$
 (24)

$$\hat{X} \otimes \hat{Y}^* = \Lambda(|\hat{X}\rangle\rangle\langle\langle\hat{Y}|). \tag{25}$$

Theorem 2 connects two relevant operators on $\mathcal{H}_d^{\otimes 2}$ having different tensor product structures, i.e., the Kronecker product $\hat{X} \otimes \hat{Y}^*$ and the dyadic product $|\hat{X}\rangle\rangle\langle\langle\hat{Y}|$. To prove the Theorem 2, we first note the following lemma.

Lemma 3 The identity operator on $\mathcal{H}_d^{\otimes 2}$ and the (unnormalized) density operator of the isotropic state on $\mathcal{H}_d^{\otimes 2}$ are related as follows.

$$|\hat{I}\rangle\rangle\langle\langle\hat{I}| = \Lambda(\hat{I}\otimes\hat{I}),$$
 (26)

$$\hat{I} \otimes \hat{I} = \Lambda(|\hat{I}\rangle\rangle\langle\langle\hat{I}|).$$
 (27)

It is straightforward to confirm Eqs. (26) and (27) by writing $|\hat{I}\rangle\rangle\langle\langle\hat{I}|$ and $\hat{I}\otimes\hat{I}$ using the standard state basis $|i\rangle$ explicitly. Then, it follows that

$$\begin{aligned} |\hat{X}\rangle\rangle\langle\langle\hat{Y}| &= (\hat{X}\otimes\hat{I})|\hat{I}\rangle\rangle\langle\langle\hat{I}|(\hat{I}\otimes\hat{Y}^*) \\ &= \Lambda((\hat{X}\otimes\hat{I})(\hat{I}\otimes\hat{I})(\hat{I}\otimes\hat{Y}^*)) = \Lambda(\hat{X}\otimes\hat{Y}^*), \end{aligned}$$

$$\begin{split} \hat{X} \otimes \hat{Y}^* &= (\hat{X} \otimes \hat{I})(\hat{I} \otimes \hat{I})(\hat{I} \otimes \hat{Y}^*) \\ &= \Lambda((\hat{X} \otimes \hat{I})|\hat{I}\rangle\rangle\langle\langle\hat{I}|(\hat{I} \otimes \hat{Y}^*)) = \Lambda(|\hat{X}\rangle\langle\hat{Y}|), \end{split}$$

where we used Eq. (5). Accordingly, Theorem 2 is proved. At this point, we note that the action of the bijection $\Lambda(\odot)$ corresponds to reshuffling of the matrix introduced by Życzkowski and Bengtsson: if we consider the matrix for the operator on $\mathcal{H}_d^{\otimes 2}$ defined with respect to the standard state basis, the mapped operator by $\Lambda(\odot)$ has a reshuffled one of the original matrix [20]. The bijection $\Lambda(\odot)$ is also closely related to the matrix realignment introduced by Chen and Wu to discuss the separability criterion for the bipartite density matrix [39]. It is easy to confirm that $\Lambda(\odot)$ is involutory, that is, $\Lambda(\Lambda(\odot)) = \odot$. It should be also noted that $\Lambda(\odot)$ does not preserve Hermiticity and the rank of the transformed operator, so its spectrum is not preserved [20]. This means that $\Lambda(\odot)$ represents a non-physical operation. It follows from Theorem 2 that $\hat{\hat{\chi}} = \Lambda(\hat{\hat{S}})$ and $\hat{\hat{S}} = \Lambda(\hat{\hat{\chi}})$, i.e., $\hat{\hat{S}}$ and $\hat{\chi}$ are bijective.

From this bijective relation, we can explore the bijection between χ - and \mathcal{S} -matrices. To this end, we expand $|\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|$ in terms of $\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*}$, and vice versa. Since they are bijective, it follows that

$$\hat{E}_{\alpha} \otimes \hat{E}_{\beta}^{*} = \Lambda(|\hat{E}_{\alpha}\rangle)\langle\langle\hat{E}_{\beta}|)$$

$$= \sum_{\alpha',\beta',\gamma=0}^{d^{2}-1} |\hat{E}_{\alpha'}\rangle\rangle\langle\langle\hat{E}_{\beta'}|M_{\alpha'\beta',\alpha\beta}, \quad (28)$$

$$|\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}| = \Lambda(\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*})$$

$$= \sum_{\alpha',\beta'=0}^{d^{2}-1}\hat{E}_{\alpha'}\otimes\hat{E}_{\beta'}^{*}(M^{\dagger})_{\alpha'\beta',\alpha\beta}, \quad (29)$$

where $M_{\alpha'\beta',\alpha\beta}$ is $\alpha'\beta';\alpha\beta$ -entry of the $d^4\times d^4$ complex matrix M. It is explicitly given as

$$M_{\alpha'\beta';\alpha\beta} = \operatorname{Tr}(|\hat{E}_{\alpha'}\rangle)\langle\langle\hat{E}_{\beta'}|)^{\dagger}\hat{E}_{\alpha}\otimes\hat{E}_{\beta}^{*}$$
$$= \sum_{\gamma=0}^{d^{2}-1} Q_{\alpha'\alpha}^{\gamma} R_{\beta\beta'}^{\gamma}, \tag{30}$$

where the coefficients

$$Q_{\alpha\beta}^{\gamma} = \langle \langle \hat{E}_{\alpha} | (\hat{I} \otimes \hat{\pi}_{\gamma}) | \hat{E}_{\beta} \rangle \rangle, \tag{31}$$

$$R_{\alpha\beta}^{\gamma} = \langle \langle \hat{E}_{\alpha} | (\hat{\pi}_{\gamma} \otimes \hat{I}) | \hat{E}_{\beta} \rangle \rangle \tag{32}$$

are the computable matrix elements of the operators $\hat{I}\otimes\hat{\pi}_{\gamma}$ and $\hat{\pi}_{\gamma}\otimes\hat{I}$ on $\mathcal{H}_{d}^{\otimes 2}$ defined with respect to the basis set $\{|\hat{E}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^{2}-1}$. These coefficients form the $d^{2}\times d^{2}$ complex matrices $Q^{\gamma}\equiv [Q_{\alpha\beta}^{\gamma}]_{\alpha,\beta=0}^{d^{2}-1}$ and $R^{\gamma}\equiv [R_{\alpha\beta}^{\gamma}]_{\alpha,\beta=0}^{d^{2}-1}$. It is easy to confirm that M is Hermitian as well as unitary, i.e., $(M^{\dagger})_{\alpha'\beta',\alpha\beta}=(M_{\alpha\beta,\alpha'\beta'})^{*}=$

 $M_{\alpha'\beta',\alpha\beta}$ and $\sum_{\alpha'',\beta''}(M^{\dagger})_{\alpha\beta,\alpha''\beta''}M_{\alpha''\beta'';\alpha'\beta'} = \sum_{\alpha'',\beta''}M_{\alpha\beta;\alpha''\beta''}(M^{\dagger})_{\alpha''\beta'',\alpha'\beta'} = \delta_{\alpha\alpha'}\delta_{\beta\beta'}$. By using these results, we obtain a bijection between the χ -and S-matrices:

$$\chi = \sum_{\gamma=0}^{d^2 - 1} Q^{\gamma} \mathcal{S} R^{\gamma}, \tag{33}$$

$$S = \sum_{\gamma=0}^{d^2-1} Q^{\gamma} \chi R^{\gamma}, \tag{34}$$

which are given by the sum of the multiplication of three known matrices Q^{γ} , χ , and R^{γ} , and evidently computable.

The above formulation can be straightforwardly extended to describe two-qudit operations. In this case, different choices of basis sets are allowed for two systems. Let us choose the set $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$ acting on the first qudit space and the set $\{\hat{F}_{\alpha}\}_{\alpha=0}^{d^2-1}$ acting on the second qudit space. The general two-qudit superoperator can be written as

$$\hat{\hat{\mathcal{S}}} = \sum_{\alpha,\beta,\gamma,\delta=0}^{d^2-1} \mathcal{S}_{\alpha\beta,\gamma\delta} |\hat{E}_{\alpha}\rangle\rangle |\hat{F}_{\beta}\rangle\rangle \langle\langle \hat{E}_{\gamma} | \langle\langle \hat{F}_{\delta} |$$
 (35)

acting on the d^4 -dimensional L-space \mathcal{L}_{d^4} as well as

$$\hat{\hat{\mathcal{S}}}(\odot) = \sum_{\alpha,\beta,\gamma,\delta=0}^{d^2-1} \chi_{\alpha\beta,\gamma\delta} \hat{E}_{\alpha} \otimes \hat{F}_{\beta} \odot \hat{E}_{\gamma}^{\dagger} \otimes \hat{F}_{\delta}^{\dagger} \qquad (36)$$

acting on \mathcal{HS}_{d^2} . These superoperators are characterized with the $d^4 \times d^4$ matrices $\mathcal{S} \equiv \left[\mathcal{S}_{\alpha\beta,\gamma\delta}\right]_{\alpha,\beta,\gamma,\delta=0}^{d^2-1}$ and $\chi \equiv \left[\chi_{\alpha\beta,\gamma\delta}\right]_{\alpha,\beta,\gamma,\delta=0}^{d^2-1}$. The bijective Choi operator is defined on the d^4 -dimensional H-space $\mathcal{H}_d^{\otimes 4}$ that is identified with the L-space \mathcal{L}_{d^4} as follows:

$$\hat{\hat{\chi}} \equiv \hat{\hat{S}}^{(13)} \otimes \hat{\hat{I}}^{(24)} (d^2 \hat{\rho}_I^{(12)} \otimes \hat{\rho}_I^{(34)}), \tag{37}$$

where the indices refer to the factors in $\mathcal{H}_d^{\otimes 4}$ in which the corresponding operations have a nontrivial action [41, 42, 43]. Then, it is straightforward to show that $\hat{\mathcal{S}}$ and $\hat{\chi}$ can be written as follows:

$$\hat{\hat{S}} = \sum_{\alpha,\beta,\gamma,\delta=0}^{d^2-1} \mathcal{S}_{\alpha\beta,\gamma\delta} |\hat{E}_{\alpha}\rangle\rangle |\hat{F}_{\beta}\rangle\rangle \langle\langle \hat{E}_{\gamma} | \langle\langle \hat{F}_{\delta} | \rangle\rangle |\hat{F}_{\beta}\rangle\rangle \langle\langle \hat{E}_{\gamma} | \langle\langle \hat{F}_{\delta} | \rangle\rangle |\hat{F}_{\delta}\rangle\rangle \langle\langle \hat{E}_{\gamma} | \langle\langle \hat{F}_{\delta} | \rangle\rangle |\hat{F}_{\delta}\rangle\rangle \langle\langle \hat{F}_{\delta} | \rangle\rangle |\hat{F}_{\delta}\rangle\rangle \langle\langle \hat{F}_{\delta} | \rangle |\hat{F}_{\delta}\rangle\rangle \langle\langle \hat{F}_{\delta} | \rangle\rangle \langle\langle$$

$$\hat{\chi} = \sum_{\alpha,\beta,\gamma,\delta=0}^{d^2-1} \chi_{\alpha\beta,\gamma\delta} |\hat{E}_{\alpha}\rangle\rangle |\hat{F}_{\beta}\rangle\rangle \langle\langle \hat{E}_{\gamma}|\langle\langle \hat{F}_{\delta}| \rangle\rangle |\hat{F}_{\delta}\rangle\rangle \langle\langle \hat{F}_{\delta}| \rangle \langle\langle \hat{F}_{\delta}| \rangle \langle\langle \hat{F}_{\delta}| \rangle \rangle \langle\langle \hat{F}_{\delta}| \rangle \langle\langle \hat{F}_{\delta}| \rangle \langle\langle \hat{F}_{\delta}| \rangle \rangle \langle\langle \hat{F}_{\delta}| \rangle \langle\langle \hat{F}$$

It follows that the two operators are certainly bijective: $\hat{\hat{\chi}} = \Lambda \otimes \Lambda(\hat{\hat{S}})$ and $\hat{\hat{S}} = \Lambda \otimes \Lambda(\hat{\hat{\chi}})$. From these bijective relations, we can explore the bijection between the χ -and S-matrices for a two-qudit operation as

$$\chi = \sum_{\gamma,\lambda=0}^{d^2-1} Q^{\gamma} \otimes S^{\lambda} \mathcal{S} R^{\gamma} \otimes T^{\lambda}, \tag{40}$$

$$S = \sum_{\gamma,\lambda=0}^{d^2-1} Q^{\gamma} \otimes S^{\lambda} \chi R^{\gamma} \otimes T^{\lambda}, \tag{41}$$

where $d^2 \times d^2$ matrices Q^{γ} and R^{γ} are given by Eqs. (31) and (32), and the matrix entries of S^{λ} and T^{λ} are given by the matrix elements of the operators $\hat{I} \otimes \hat{\pi}_{\gamma}$ and $\hat{\pi}_{\gamma} \otimes \hat{I}$ on $\mathcal{H}_d^{\otimes 2}$ defined with respect to the basis set $\{|\hat{F}_{\alpha}\rangle\rangle\}_{\alpha=0}^{d^2-1}$:

$$S_{\alpha\beta}^{\gamma} = \langle \langle \hat{F}_{\alpha} | (\hat{I} \otimes \hat{\pi}_{\gamma}) | \hat{F}_{\beta} \rangle \rangle, \tag{42}$$

$$T_{\alpha\beta}^{\gamma} = \langle \langle \hat{F}_{\alpha} | (\hat{\pi}_{\gamma} \otimes \hat{I}) | \hat{F}_{\beta} \rangle \rangle. \tag{43}$$

We can further extend the above formulation to describe n-qudit operations. In this case, the bijective relation between $\hat{\hat{S}}$ and $\hat{\hat{\chi}}$ reads $\hat{\hat{\chi}} = \Lambda^{\otimes n}(\hat{\hat{S}})$ and $\hat{\hat{S}} = \Lambda^{\otimes n}(\hat{\hat{\chi}})$. By using these relations, we can straightforwardly extend Eqs. (40) and (41) to the bijection between the χ - and S-matrices for an n-qudit operation.

It is obvious that not all the space of χ - and \mathcal{S} -matrices corresponds to physically realizable operations. For example, we can describe an anti-unitary operation by using the χ - and \mathcal{S} -matrices, which is evidently an unphysical operation. The requirement for the χ - and \mathcal{S} -matrices to represent physical quantum operations has been extensively studied by many researchers. In the following, the requirements common for the single- and two-qudit operations are summarized [21].

Condition 1 (Hermiticity) The physical quantum operation \mathfrak{S} should preserve Hermiticity; i.e., \mathfrak{S} maps any Hermite operator into an Hermite operator.

Condition 2 (Positivity) The physical quantum operation \mathfrak{S} should be positive; i.e., \mathfrak{S} maps any positive operator into an positive operator.

Condition 3 (Complete positivity) The physical quantum operation $\mathfrak S$ should be completely positive; i.e., positivity is preserved if we extend the L-space and HS-space by adding more qudits. That is, the superoperator $\hat{\mathcal S} \otimes \hat{\mathcal I}$ on the extended spaces should be positive.

It is known that 3 is sufficient for 1 and 2, and 2 is sufficient for 1. Therefore, we require complete positivity for a physical quantum operation. Complete positivity can be expressed as a particularly simple condition for the χ -matrix.

Theorem 3 The linear operation \mathfrak{S} is completely positive, iff the χ -matrix is positive.

This is natural on physical grounds, because the Choi operator $\hat{\chi}$ should be an unnormalized density operator associated with the system which was subjected to the quantum operation as will be discussed in the next section. In addition to 3, any physical quantum operation should satisfy the following condition.

Condition 4 (Trace non-increasing) The physical quantum operation \mathfrak{S} should be trace non-increasing; i.e., the mapped operator should have trace less than one.

This condition is simply expressed as the restriction on the χ -matrix: $\text{Tr}_1\chi \leq I^{(1)}$ for a single-qudit operation and $\text{Tr}_{13}\chi \leq I^{(2)}$ for a two-qudit operation, where $I^{(n)}$ is an identity matrix with size d^n .

It is needless to say that the χ - and S-matrices can be defined with respect to arbitrary operator basis sets. Once these matrices are given with respect to a particular operator basis set, they can be converted into those defined with respect to the other basis set. It is obvious from Eqs. (19), (20), (39), and (38) that the two matrices defined with respect to different bases are unitarily equivalent. To be specific, let χ^E and S^E be the χ - and S-matrices for a single-qudit operation defined with respect to the operator basis set $\{\hat{E}_{\alpha}\}_{\alpha=0}^{d^2-1}$, and χ^F and S^F be those defined with respect to the operator basis set $\{\hat{F}_{\alpha}\}_{\alpha=0}^{d^2-1}$, where the two bases are unitarily related as shown in Eqs. (15) and (16). Then, these matrices should be written as

$$S^F = \mathcal{U}^{\dagger} S^E \mathcal{U}, \tag{44}$$

$$\chi^F = \mathcal{U}^{\dagger} \chi^E \mathcal{U}, \tag{45}$$

where $\mathcal{U} \equiv \left[\mathcal{U}_{\alpha\beta}\right]_{\alpha=0}^{d^2-1}$ is a $d^2 \times d^2$ unitary matrix. For the case of two-qudit operation, we need to extend the set of the operator basis to cover all the possible basis sets defined for the two-qudit operator space, that is, one that is a factorable set as well as not a factorable set with respect to the first and second systems. The general set of operator basis $\{\hat{\Phi}_{\gamma}\}_{\gamma=0}^{d^4-1}$ on $\mathcal{H}_d^{\otimes 2}$ should be unitarily related to the factorable operator bases $\hat{E}_{\alpha} \otimes \hat{F}_{\beta}$. If we introduce a $d^4 \times d^4$ unitary matrix $\mathcal{U} \equiv \left[\mathcal{U}_{\alpha\beta}\right]_{\alpha=0}^{d^4-1}$ that relates $\hat{\Phi}_{\gamma}$ and $\hat{E}_{\alpha} \otimes \hat{F}_{\beta}$:

$$\hat{\Phi}_{\gamma} = \sum_{\alpha,\beta=0}^{d^2-1} \hat{E}_{\alpha} \otimes \hat{F}_{\beta} \mathcal{U}_{[\alpha,\beta]\gamma}, \tag{46}$$

where $[\alpha, \beta] := d^2\alpha + \beta$, it follows that Eqs. (44) and (45) also hold for two-qudit operations.

The χ - and S-matrices can be diagonalized by choosing the appropriate operator basis sets, but are not necessarily diagonalized simultaneously by a unique set. The operator basis set that diagonalizes the χ -matrix, each element of which is multiplied by the square root of the associated eigenvalue, forms a particular set of Kraus operators in the Kraus form of the quantum operation. Any set of Kraus operators can be obtained by noting the unitary freedom in the Kraus form [2]. It follows from Eqs. (19), (20), (39), and (38) that the same operator basis set with the associated set of eigenvalues also gives an operator-Schmidt decomposition for the L-space superoperator $\hat{\mathcal{S}}$ [20]. Therefore, the Kraus rank for the HS-space superoperator $\hat{\mathcal{S}}$ (\odot) and Schmidt number of the L-space superoperator $\hat{\mathcal{S}}$ must be equal.

IV. APPLICATIONS OF χ - AND S-MATRICES

This section presents the several applications of the χ and S-matrices. We discuss how these matrices and the
present formulation are useful for analysis and design of
quantum operations.

Experimental identification of quantum operations

In the first example, we explain how useful the present formulation is for experimental identification of quantum operations [6, 7, 8, 9, 10, 11, 12]. This task is important because the development of any quantum device or circuit for quantum computation and communication, which can be considered as an input-output system that performs an intended quantum operation on its input state and transforms it into its output state, necessarily requires experimental benchmarking of its performance. The identification of a two-qudit device is particularly interesting from a practical viewpoint as well as a scientific one because it may involve a nonseparable operation which has a purely quantum mechanical nature, i.e., it cannot be simulated by using any classical method.

Identification of an input-output system amounts to identifying its χ - or S-matrix, since these matrices characterize the system in question completely as far as input and output data are concerned. The evaluated matrices should reproduce the behavior of the system well enough when the system is stimulated by any class of inputs of interest, and they should be useful for engineering the system of interest, e.g., to permit control of the system, to allow transmission of information through the system, to yield predictions of future behavior, etc. Identification problems are commonly regarded as inversion problems, where the χ - or S-matrix is to be statistically estimated from incomplete prior knowledge of the system, using prior knowledge of corresponding inputs and the collection of data obtained by measurement of outputs that usually contain noise. In what follows, it will be shown that this common belief is not the case for identification of quantum operations. To be specific, we can estimate both the χ - and S-matrices without any inversion procedure if we can make use of an entangled resource and a sequence of local measurements assisted by classical communication [7, 9, 11, 31, 42].

Consider first the identification of a single-qudit operation. Equations (19) and (20) show that all the elements of the χ - and S-matrices are given by the expansion coefficients of the operators $\hat{\hat{\chi}}$ or $\hat{\hat{\mathcal{S}}}$ with respect to two different types of operator basis on $\mathcal{H}_d^{\otimes 2}$. Of these two operators, the Choi operator $\hat{\chi}$ is particularly useful since it is a positive operator associated with the physical state of the bipartite object. To be specific, it can be interpreted as the unnormalized output state from the system in question where qudit 1 of the two qudits prepared in an isotropic state is input into the system and undergoes the quantum operation \mathfrak{S} while qudit 2 is left untouched. Therefore, we can prepare the output state corresponding to the normalized Choi operator $\hat{\chi}/d \equiv \hat{\mathcal{S}} \otimes \hat{\mathcal{I}}(\hat{\rho}_I)$ with the use of several copies of the isotropic-state input for the two qudits. Thus, the identification of a single-qudit operation reduces to the identification of a two-qudit state. It follows from Eq. (22) that every element of the Smatrix can be directly obtained by determining the expectation value of the corresponding product operator basis $\langle \hat{E}_{\alpha} \otimes \hat{E}_{\beta}^* \rangle$ for the output states after the quantum operation has taken place. If the basis \hat{E}_{α} is chosen to be the Hermitian operator basis $\hat{\lambda}_{\alpha}$, it suffices to make a set of d^4 -independent local measurements assisted by classical communication to determine the whole set of the real expectation values $\langle \hat{\lambda}_{\alpha} \otimes \hat{\lambda}_{\beta} \rangle$. Accordingly, we can obtain the S-matrix defined with respect to the Hermitian operator basis set $\{\hat{\lambda}_{\alpha}\}_{\alpha=0}^{d^2-1}$. Once the S-matrix is obtained, it is easy to convert it to the χ -matrix defined with respect to the same basis by using Eqs. (31)-(33) and also into the χ - and S-matrices defined with respect to the arbitrary chosen basis by using Eqs. (44) and (45).

The identification of a two-qudit operation can be carried out in the same way as the identification of a single-qudit operation. In this case, we prepare the state corresponding to the Choi operator in Eq. (37) with the use of several copies of the product of isotropic states prepared in the four qudits. To prepare the output state, we initially prepare the product of isotropic states $\hat{\rho}_I^{(12)}\otimes\hat{\rho}_I^{(34)}$ in two pairs of two qudits (qudits 1-2 and qudits 3-4). Then qudit 1 and qudit 3 are input into the system in question, undergo the quantum operation \mathfrak{S} jointly while the other qudits are left untouched. This setup leads to an output state $\hat{\chi}/d^2$ in four-qudits. Thus, the identification of a two-qudit operation reduces to the identification of a four-qudit state. It follows from Eq. (38) that every element of the S-matrix for the two-gudit operation can be directly obtained by determining the real expectation value of the corresponding product operator basis $\langle \hat{\lambda}_{\alpha} \otimes \hat{\lambda}_{\gamma} \otimes \hat{\lambda}_{\beta} \otimes \hat{\lambda}_{\delta} \rangle$ for the output states after the quantum operation has taken place, if all the relevant basis sets are chosen to be the Hermitian operator basis $\hat{\lambda}_{\alpha}$. It suffices to make a set of d^{8} -independent local measurements assisted by classical communication

to determine the whole set of real expectation values $\langle \hat{\lambda}_{\alpha} \otimes \hat{\lambda}_{\gamma} \otimes \hat{\lambda}_{\beta} \otimes \hat{\lambda}_{\delta} \rangle$. Accordingly, we can obtain the S-matrix defined with respect to the Hermitian operator basis $\{\hat{\lambda}_{\alpha} \otimes \hat{\lambda}_{\beta}\}_{\alpha,\beta=0}^{d^2-1}$. The S-matrix can be converted into the χ -matrix by using Eqs. (40)-(43). The S-and χ -matrices defined with respect to arbitrary chosen bases can be obtained by applying the appropriate matrix unitary transformation.

Matrix analysis of quantum operations

This section discusses in what way the χ - and \mathcal{S} -matrices contribute to developing quantum devices and circuits for quantum computation and communication. We consider two classes of applications in which these matrices offer useful mathematical models for quantum operations. The first one concerns physical and information theoretic analysis of quantum operations and the other concerns a logical calculus of quantum circuits or algorithms comprised of a sequence of quantum operations.

Let us first consider the physical and information theoretic analysis of quantum operations. For this purpose, it is preferable to use the χ -matrix. This stems partly from the fact that the χ -matrix is positive and isomorphic to the density matrix in the doubled Hilbert space. Physically, the diagonal elements of the process matrix show the populations of, and its off-diagonal elements show the coherences between, the basis operators making up the quantum operation, analogous to the interpretation of density matrix elements as populations of, and coherences between, basis states. Owing to Jamiolkowski isomorphism, the dynamic problems concerning quantum operations can be turned into kinematic problems concerning quantum states in a higher dimensional space, and one can make use of a well-understood statebased technique for analyzing the quantum operation. In what follows, we show several illustrative examples and interesting problems from the physical and information theoretic viewpoints.

The first example concerns the fidelity or distance measure between two quantum operations. Several measures that make use of the above isomorphism have been proposed to quantify how close the quantum operation in question is to the ideal operation (usually a unitary operation) we are trying to implement. For example, the state fidelity defined between two states is extended to compare the two operations. The process fidelity F_p is defined by using the χ -matrix $\tilde{\chi}$ of the system in question and the rank one χ -matrix χ_{ideal} of the ideal system in the state-fidelity formula, that is, $F_p = \frac{1}{d^{2n}} \text{Tr} \tilde{\chi} \chi_{ideal}$, where $n{=}1$ for single-qudit operation and $n{=}2$ for a twoqudit operation. The average gate fidelity \bar{F} defined as the state fidelity between the output state after the quantum operation and the ideal output can be calculated from the process fidelity. The purity defined for the density matrix can be extended to characterize how much of a mixture the quantum operation introduces, which is also represented by the simple function of the χ -matrix of the system in question [10, 18, 44, 45].

The next example concerns the analysis of a quantum operation acting on the composite system. As mentioned before, the χ -matrix of a two-qudit operation is interesting from a practical as well as a scientific viewpoint. The Jamiolkowski isomorphism for a two-qudit operation (Eqs. (37) and (38)) implies that the notion of entanglement can be extended from quantum states to quantum operations. Analogously to what happens for states, quantum operations on a composite system can be entangled [46, 47]. A quantum operation acting on two subsystems is said to be separable if its action can be expressed in the Kraus form

$$\hat{\mathcal{S}}(\odot) = \sum_{i} (\hat{A}_{i} \otimes \hat{B}_{i}) \odot (\hat{A}_{i} \otimes \hat{B}_{i})^{\dagger}, \tag{47}$$

where \hat{A}_i and \hat{B}_i are operators acting on each subsystem [48, 49, 50]. Otherwise, we say that it is nonseparable (or entangled). Quantum operations that can be performed by local operations and classical communications (the class of LOCC operations) are described by separable quantum operations, yet there are separable quantum operations that cannot be implemented with LOCC operations with probability one [41, 43, 51]. Anyway, these are useless for creating entanglement in an initially unentangled system. It has been pointed out by several authors that the separability and entangling properties of quantum operations acting on two systems can be discussed in terms of the Choi operator for two-qudit operations (Eq. (38)) [41, 42, 43]. In the present context, this reduces to discussing the separability properties of the γ -matrices. For example, there is a condition for the χ -matrix equivalent to Eq. (47): a quantum operation acting on two subsystems is separable if its χ -matrix can be written as $\chi = \sum_i \chi_i^{(A)} \otimes \chi_i^{(B)}$, where $\chi_i^{(A)}$ and $\chi_i^{(B)}$ are the χ -matrices for the quantum operation acting on each subsystem. Thus, the separability of general quantum operations acting on the composite system is reduced to the separability of its χ -matrix. Since the separability criterion and measure for the general $d^4 \times d^4$ positive matrix is not fully understood, it remains as an important problem for quantum information science to find such a criterion and measure for general two-qudit quantum operations.

Let us turn our attention to a logical calculus of quantum circuits or algorithms. For this purpose, the \mathcal{S} -matrix is practically useful. This follows from the fact that L-space superoperator algebra works just like Dirac operator algebra. For example, consider the scenario in which two-quantum operations \mathfrak{S}_1 and \mathfrak{S}_2 act sequentially on a quantum system. Assume that the associated \mathcal{S} -matrices are given with respect to the same operator basis set $\{|\hat{E}_{\alpha}\rangle\}_{\alpha=0}^{N-1}$ in \mathcal{L}_N , where $N=d^2$ for single-qudit operation and $N=d^4$ for two-qudit operation. Then the composite operation $\mathfrak{S}=\mathfrak{S}_1\circ\mathfrak{S}_2$ is described

by the multiplication of L-space superoperators

$$\hat{\hat{\mathcal{S}}} = \hat{\hat{\mathcal{S}}}_1 \hat{\hat{\mathcal{S}}}_2 = \sum_{\alpha,\beta=0}^{N-1} \mathcal{S}_{\alpha\beta} |\hat{E}_{\alpha}\rangle\rangle\langle\langle\hat{E}_{\beta}|, \tag{48}$$

where

$$S_{\alpha\beta} = \sum_{\gamma=0}^{N-1} (S_1)_{\alpha\gamma} (S_2)_{\gamma\beta}.$$
 (49)

The extension to the case in which a sequence of a finite number of quantum operations is applied to the same quantum system is trivial. Equation (49) implies that the S-matrix of the composite operation reduces to the multiplication of the S-matrices of the individual operations. This makes it practically advantageous using the S-matrix to make a logical calculus of quantum circuits or algorithms comprised of a sequence of elementary single-and two-qudit quantum operations.

Consider next the quantum circuit or algorithm comprised of a sequence of quantum operations each of which acts not necessarily on the same quantum system. This offers a general model for the quantum circuit acting on the large numbers of qudits [3]. To analyze and design such a quantum circuit, we need to consider quantum operations acting on the whole set of qudits and associated extended S-matrix. Such an extended S-matrix is non-trivial, but its bijective χ -matrix is trivially obtained by taking the tensor product with identity matrix, that is, the χ -matrix for the identity operation on the irrelevant system. If the χ -matrix for the quantum operation \mathfrak{S} on the relevant space is given by χ , the χ -matrix for the extended quantum operation is given by $\chi \otimes I$. On the other hand, we can trivially extend the conversion formulas (40) and (41) to those formulas for the quantum operation acting on more qudits. Therefore, we can calculate the extended S-matrix for each quantum operation from the associated S-matrix for the quantum operation acting on the relevant space. The S-matrix for a sequence of operations acting on the space of the whole quantum systems can be calculated by multiplication of the extended S-matrices for the individual quantum operations.

The S-matrix analysis of the quantum operation has the following potential advantage. It can deal with a non-unitary operation in which mixed state evolution occurs. Noisy quantum operation, probabilistic subroutines, measurements, and even trace-decreasing quantum filters can be treated. This is in contrast to the usual analysis based on unitary matrix which can deal only with unitary gate in which only the pure state evolution is allowed. It thus offers us an mathematical model to analyze and design the logical operation of wider range of the complex quantum circuits and algorithms [3].

In the above discussion, we considered two applicational classes, i.e., physical and information theoretic analysis and logical calculus of quantum operations, in which the χ - and \mathcal{S} -matrices matrices offer useful mathematical models. They have their own useful applications.

The present formulation will offer us the way of building bridges across the two applicational classes. For example, the entangling properties of the quantum circuits comprised of a sequence of single- and two-qudit quantum operations acting on several qudits can be discussed. The present formulation will also help us to analyze and benchmark the quantum operation realized in the actual device.

V. CONCLUSIONS

We have considered two matrix representations of single- and two-qudit quantum operations defined with respect to an arbitrary operator basis, i.e., the χ and S-matrices. We have provided various change-ofrepresentation formulas for these matrices including bijections between the χ - and S-matrices. These matrices are defined with the expansion coefficients of two operators on a doubled Hilbert space, that is, the L-space superoperator and the Choi operator. These operators are mutually convertible through a particular bijection by which the Kronecker products of the relevant operator basis and the dyadic products of the associated state basis are mutually converted. From this fact, the mutual conversion formulas between two matrices are established as computable matrix multiplication formulas. Extention to multi-qudit quantum operation is also trivial. These matrices are useful for their own particular classes of applications, which might be interesting from a practical as well as a scientific point of view.

We have presented possible applications of the present formulation. By using the present formulation, an experimental identification of a quantum operation can be reduced to determining the expectation values of a Hermitian operator basis set on a doubled Hilbert space. This can be done if we prepare several copies of the isotropicstate input or the product of isotropic states input. By using the χ -matrix, we can make a physical as well as a quantum information theoretic characterization of the quantum operation. In particular, the χ -matrix is useful to discuss the entangling properties of the quantum operation acting on the composite system, since the problem of the separability of the quantum operation is reduced to the problem of the separability of the χ -matrix. On the other hand, the S-matrix is useful when we discuss the typical quantum circuit comprised of a sequence of single- and two-qudit quantum operations each of which acts on different quantum qubits. It is possible by considering the extended S-matrix of each quantum operation acting on the whole state space of the relevant qudits. Such extended S-matrices can be calculated from the associated, bijective γ -matrices by taking the tensor product with the appropriate identity matrix. Accordingly, we can calculate the S-matrix for a quantum circuit by multiplying the extended S-matrices of each operation. This should be very useful to analyze and design a wide range of the quantum circuits and algorithms involving non-unitary operation.

We thank Satoshi Ishizaka and Akihisa Tomita for their helpful discussions. This work was supported by the CREST program of the Japan Science and Technology Agency.

- K. Kraus, States Effects and Operations: Fundamental Notions of Quantum Theory, Lecture Notes in Physics Vol. 190 (Springer-Verlag, Berlin, 1983).
- [2] M.A. Nielsen, I.L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Oxford, 2000).
- [3] D. Aharonov, A. Kitaev, and N. Nisan, e-print quant-ph/9806029.
- [4] P. Stelmachovič and V. Bužek, Phys. Rev. A 64, 062106 (2001); 67, 029902(E) (2003).
- [5] H. Hayashi, G. Kimura, and Y. Ota, Phys. Rev. A 67, 062109 (2003).
- [6] Y. Nambu et al., Proc. SPIE Int. Soc. Opt. Eng. 4917, 13 (2002).
- [7] J. B. Altepeter et al., Phys. Rev. Lett. 90, 193601 (2003).
- [8] M. W. Mitchell, C. W. Ellenor, S. Schneider, and A. M. Steinberg, Phys. Rev. Lett. 91, 120402 (2003).
- [9] F. De Martini et al., Phys. Rev. A 67, 062307 (2003).
- [10] J. L. O'Brien et al., Phys. Rev. Lett. 93, 080502 (2004).
- [11] V. Secondi, F. Sciarrino, and F. De Martini, Phys. Rev. A 70, 040301(R) (2004).
- [12] Y. Nambu and K. Nakamura, Phys. Rev. Lett. 94, 010404 (2005).
- [13] C. M. Caves, J. Superconductivity 12, 707 (1999).
- [14] V.E. Tarasov, J. Phys. A. 35, 5207 (2002).
- [15] L. P. Hughston, R. Jozsa, and W. K. Wootters, Phys. Lett. 183, 14 (1993).
- [16] G. M. D'Ariano, P. Lo Presti, and M. F. Sacchi, Phys. Lett. A 272, 32 (2000).
- [17] I. L. Chuang and M. A. Nielsen, J. Mod. Opt. 44, 2455 (1997).
- [18] A. G. White et.al., e-print quant-ph/0308115.
- [19] E. C. G. Sudarshan, P. M. Mathews, and J. Rau., Phys. Rev., 121, 920 (1961).
- [20] K. Życzkowski and I. Bengtsson, Open Syst. Inf. Dyn. 11, 3-42 (2004).
- [21] P. Arrighi and C. Patricot, Annals Phys. **311**, 26 (2004).
- [22] K. Blum, Density Matrix Theory and Applications (Plenum Press, New York, 1981).
- [23] A. Royer, Phys. Rev. A 43, 44 (1991); 45, 793 (1992).
- [24] S. W. Hawking, Phys. Rev. D 14, 2460 (1976).
- [25] R. M. Wald, Phys. Rev. **D** 21, 2742 (1980).
- [26] A. Fujiwara and P. Algoet, Phys. Rev. A 59, 3290 (1999).
- [27] A. Ben-Reuven, Phys. Rev. **141**, 34 (1966).

- [28] A. Ben-Reuven, Adv. Chem. Phys. 33, 235 (1975).
- [29] A. Ben-Reuven, Phys. Rev. **A 22**, 2572 (1980); **22**, 2585 (1980).
- [30] Y. Prior and A. Ben-Reuven, Phys. Rev. A 33, 2362 (1986).
- [31] G. M. D'Ariano, and P. Lo Presti, Phys. Rev. Lett. 86, 4195 (2001); 91, 47902 (2003).
- [32] M. Horodecki and P. Horodecki, Phys. Rev. A 59, 4206 (1999).
- [33] B. M. Terhal and K. G. H. Vollbrecht, Phys. Rev. Lett. 85, 2625-2628 (2000).
- [34] G. Mahler and V. A. Weberruß, Quantum Networks: Dynamics of Open Nanostructures, 2nd ed. (Springer, New York, 1998).
- [35] C. Miquel, J. P. Paz, and M. Saraceno, Phys. Rev. A 65, 062309 (2002).
- [36] M. L. Aolita, I. García-Mata, and M. Saraceno, Phys. Rev. A 70, 062301 (2004).
- [37] M.-D. Choi, Linear Algebr. Appl. 10, 285 (1975).
- [38] A. Jamiołkowski, Linear transformations which preserve trace and positive semidefiniteness of operators, Rep. Math. Phys. 3, 275 (1972).
- [39] K. Chen, and L-A.Wu, Phys. Lett. 306, 14 (2002); Quantum Info. Comp., 3 193 (2003).
- [40] T. F. Havel, J. Math. Phys. 44, 534 (2003).
- [41] J. I. Cirac, W. Dür, B. Kraus, and M. Lewenstein, Phys. Rev. Lett. 86, 544 (2001).
- [42] W. Dür and J. I. Cirac, Phys. Rev. A 64, 12317 (2001).
- [43] A. W. Harrow and M. A. Nielsen, Phys. Rev. A 68, 12308 (2003).
- [44] M. Raginsky, Phys. Lett. A 290, 11 (2001).
- [45] A. Gilchrist, N. K. Langford, and M. A. Nielsen, e-print quant-ph/0408063.
- [46] P. Zanardi, Phys. Rev. A 63, 040304(R) (2001).
- [47] X. Wang and P. Zanardi, Phys. Rev. A 66, 044303 (2002).
- [48] V. Vedral, M.B. Plenio, M.A. Rippin, and P.L. Knight, Phys. Rev. Lett. 78, 2275 (1997).
- [49] H. Barnum, M.A. Nielsen, and B.W. Schumacher, Phys. Rev. A 57, 4153 (1998).
- [50] E. M. Rains, Phys. Rev. A 60, 173 (1999).
- [51] C.H. Bennett, D.P. DiVincenzo, C.A. Fuchs, T. Mor, E. Rains, P.W. Shor, J.A. Smolin, and W.K. Wootters, Phys. Rev. A 59, 1070 (1999).